MATRL 218: Assignment 4

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1. Sketch the bond valence net for the cubic ($Pm\bar{3}m$) perovskite $Ba^{2+}Zr^{4+}(O^{2-})_3$. If the cubic cell parameter is 4.197 Å, then calculate the bond valence sums on Ba, Zr, and O. Use B = 0.37 Å and the following R_0 values: For the Ba^{2+}/O^{2-}, it is 2.285 Å and for Zr^{4+}/O^{2-} 1.928 Å. Does this suggest that $BaZrO_3$ is happy being cubic?

2. With this assignment is the VESTA file of the real structure of perovskite $CaZrO_3$. What is the crystal system? Why do you think this compound is not cubic? What is the "real" coordination of Ca^{2+} in this compound?

3. The Lennard-Jones potential for a monoatomic system is:

$$U(r) = 4\epsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right]$$

   Where ϵ is the well depth and σ is the atomic (or particle) diameter. (i) Sketch the distance-dependence of this potential using scaled units, *ie.* set $\sigma = 1$ and $\epsilon = 1$. Approximately how many atomic diameters does one need to be separated by before there is effectively no interaction. (ii) Determine by setting $\partial U(r)/\partial r = 0$, the value of r/σ for which the potential is minimum.

4. Why do you expect the dispersion (van der Waals) attraction between larger noble gas atoms to be larger than for smaller ones.

5. Sketch two interpenetrating square lattices, whose origins are separated by $(0.5, 0.5)$, and assign atoms at the corners of the two lattices with opposite charges (a "2D CsCl"). Can you write out the first few terms of the geometric Madelung constant for the above lattice. Does it look like you can sum it up to ∞.

6. Determine the Madelung constant for a 1D lattice of opposite charges.